REQUIREMENTS FOR HIGH QUALITY X-RAY SPECTROSCOPY IN AN EXPLORER CLASS MISSION

Webster C. Cash, Jr.

Laboratory for Atmospheric and Space Physics
University of Colorado
Boulder, Colorado 80309

ABSTRACT

Through the use of simulated x-ray spectra we address the question of instrument requirements for a spectrograph that could significantly advance x-ray astronomy. We conclude that resolution ($\lambda/\Delta\lambda$) in the range of 200-500, and effective collecting area in excess of 200 cm^2 are required. We present one design, based on the objective reflection grating concept, which would meet these stringent requirements in an Explorer class mission.

I. INTRODUCTION

In the last meeting of this nature, the Workshop on Compact Galactic Sources, Rappaport (1979) gave a brief overview of x-ray astronomy in terms of the three major disciplines: imaging, spectroscopy and timing. At that time, with the Einstein Observatory starting operations, x-ray imaging had reached a level of maturity far beyond that of timing or spectroscopy. The workshop concluded that an X-ray Timing Explorer was the next logical step to balancing the advance of x-ray astronomy. But, the decision to pursue timing at the expense of spectroscopy was made on technological and budgetary grounds; we know how to build a timing experiment faster and cheaper than a spectroscopy experiment. Now, with XTE in the Explorer queue, our attention must turn to spectroscopy if new scientific domains are to be opened.

The history of astrophysics also supports the argument that spectroscopy must be next. Optical astronomy did not evolve into astrophysics until well into this century, when high quality photographic spectroscopy was developed and the results interpreted through modern physics. At the turn of the century, optical astronomy was in a situation very similar to the current status of x-ray astronomy. The first concave grating spectrograph of the sun, obtained by Rowland (1882), showed an amazing wealth of information. The Solar Maximum Mission is currently showing us a fabulous array of x-ray spectral features in the sun. Yet, following Rowlands solar spectrum, there was a delay of more than twenty years before observatories became sufficiently sensitive to study stars with high resolution. In that same period imaging became quite advanced: The first photographic surveys of the sky were completed, and extragalactic astronomy was born through the discovery of vast numbers of nebulae. Simultaneously, timing studies were advancing with the quantitative studies of eclipsing

variables and novae. The problem with spectroscopy was that the bright sources in the sky were, to first order, simple blackbodies, while the objects with exotic spectra were too faint to observe.

Today, we know from low resolution x-ray spectroscopy that the brightest sources in the sky have, to first order, featureless continua , while many of the fainter sources have quite exotic spectra. The pursuit of very high resolution spectroscopy of bright sources, and adequate resolution spectroscopy of faint sources, is still the primary concern of optical astronomers. Over ninety percent of all observing time on the world's major telescopes is dedicated to spectroscopy. I think in the future it will be the same for x-ray astronomy.

In this talk I will address primarily the question of what performance level is needed before x-ray spectroscopy will mature. I will finish with my suggestion of how the necessary performance level can be achieved.

II. A SIMULATED X-RAY SPECTRUM

The quality of a spectrum, and hence the quality of science derived from it, depends on a variety of factors in the spectrograph and in the source. The performance of a spectrograph is mainly determined by spectral resolution and collecting area, while bandpass and noise characteristics play lesser roles. Since the spectrograph must be able to clearly detect the targeted spectral features, so the brightness of the source, as well as the size and shape of its spectral features play a central role in determining the spectrograph design.

To investigate the interplay between spectrograph design and source characteristics I have performed a simple computer simulation. With the help of Mike Shull, I have created a synthetic spectrum containing many of the x-ray

spectral features we know should be present. Then, by smoothing the spectrum I could determine the resolution necessary to locate, separate, and identify typical features. By introducing varying amounts of Poisson noise, I could determine how many photons are needed to make the features statistically significant. Through this exercise I have reached some conclusions that I believe are convincing.

III. RESOLUTIONS

The initial spectrum entered in the computer was an array one thousand elements long, with each bin of 2eV width. Thus, the spectrum extended up to 2 keV. By doing a simple boxcar smooth, I was able to simulate lower resolution spectra.

The series of smoothings is shown in Figure 1. Part (a) shows the spectrum smoothed to 280eV, typical of a proportional counter. The spectrum is devoid of features. Pulse height spectra such as these were obtained with HEAO-1, and through a clever inversion technique found the O absorption edge in the Crab and Sco X-1 (Kahn and Blissett, Charles et al., Kahn et al).

Moving to Figure 1(b) we see a smooth spectrum with a ledge at the position of the oxygen edge. It has a resolution of 180eV, similar to that of the SSS on Einstein, although the SSS was not able to observe below about 600eV.

Tripling the resolution (to 64eV) in 1(c) produces a dramatic difference. The absorption dip at the O edge is clearly delineated, and an emission line has appeared at the position of the Fe L lines. Figure 1(d) doubles the resolution again, with the effect of sharpening the emission line and hinting at structure in the O edge.

In Figure 1(e), where the resolution is 16eV (comparable to the OGS on Einstein), the structure in the O edge has clearly become an absorption line

at the position of the O VIII Lyman α line. The iron line is starting to show structure.

The next doubling of resolution, to 8eV, brings with it the resolution of the iron line into a complex of closely spaced lines. Also visible for the first time is the fact that the intensity drop across the O edge is not a single step. Several ionized species of oxygen are contributing to the edge.

At a resolution of 4eV in Figure 1(g) the last hidden feature emerges. A weak absorption line at the position of the O VIII Lyman α line is visible.

The last part, Figure 1(h), shows the original spectrum with full 2eV resolution. It now shows the O VIII absorption line to be saturated; the Fe line complex is fully resolved.

With each improvement in resolution we discovered new features in the spectrum until, in the last two graphs, all of the original features were apparent. By pushing the resolution beyond 2eV one could study emission and absorption line profiles, but this would require resolution of nearly 0.2eV. Since we currently don't even know the gross spectral features of x-ray sources, talk of observing line profiles seems a little absurd - that should be left for the following generation of spectroscopy. In short, 2ev resolution will be enough to discover and classify features, but little extra will be gained until resolution is almost an order of magnitude higher.

Converting to the more conventional spectroscopy notation,

$$R = \frac{\lambda}{\delta\lambda} = \frac{E}{\delta E} = \frac{500\text{eV}}{2\text{eV}} = 250.$$

IV. POISSON NOISE

In spectroscopy as in imaging, Poisson noise is the great enemy of the x-ray astronomer. Our experiment must collect enough photons in each spectral

resolution bin to make the bin-to-bin variations (which carry the information) sufficiently small. To investigate this effect, I have taken the same synthetic spectrum at full resolution and run a Poisson randomizer over it with various scale factors. The results are displayed in Figure 2. Taking the figure part by part:

a. This is a minimal spectrum, typically two photons per bin, with a total of 1281 counts in the spectrum. Nothing is visible except the overall shape of the curve, an exponential with an interstellar cutoff.

b. With 10 c/bin we start to see the O edge.

c. At 30 c/bin the O edge is clear. The O VIII Ly α is becoming statistically significant.

d. With 100 c/bin the spectrum is looking fairly good. Most of the major features are visible. The biggest problem is that, while it is clear that the features are present, quantitative statements about their size will be inaccurate.

e. This is an excellent spectrum. With 1000 c/bin all the features are clear, and quantitative assessment is clearly possible.

f. At 10^4 c/bin there is virtually no difference between the original and the randomized spectra.

From Figure 2 we have learned that a spectrum with less than 100 c/bin is inadequate while in most cases 10^4 c/bin is more than is required. A good number to shoot for is 1000 c/bin, and a barely adequate spectrum is 100 c/bin. I recommend that the Explorer be able to obtain 100-1000 c/bin in a reasonable period of time on all prime sources.

The situation is different when emission line sources are considered. Take the case of the synthetic emission line spectrum shown in Figure 3(a). When these lines are Poisson randomized we find that far fewer photons are

required. Figure 3(b) is the same spectrum with a total of only 46 photons, rebinned into 80 bins to best show the data. It is a fair representation of the original spectrum. Figure 3(c) is a similar spectrum with 188 photons. In 3(d) we have 830 photons and in 3(e), 55,000 photons. It is clear that in order to retrieve the basic physics of a line source, only 100 photons per line are needed. A total of 10^4 photons should show all the major features in a line source. This compares to the 10^5 to 10^6 photons required for a good spectrum of a continuum source. It is particularly good news for the studies of stellar coronae and supernova remnants.

V. COLLECTING AREA

Starting with the level of statistics recommended in the previous section, we can derive the needed spectrograph collecting area. With an Explorer, a typical observation should be completed in 2×10^4 seconds of exposure. In real terms this requires an entire day. In this amount of time we require enough collecting area to observe a large number of sources from many classes. This diversity of application is necessary if the Explorer is to make a major contribution to astronomy.

In Table I we list the four most prominent classes of x-ray point sources: the x-ray binaries, stellar coronae, Seyfert galaxies, and quasars. We would like to be able to observe ten or more objects in each of these classes, so we have listed the approximate flux (in HEAO-2 IPC counts) of the tenth brightest member of each class in column 2. In column 3 this flux has been converted to ph $cm^{-2}s^{-1}bin^{-1}$, except in the case of stellar coronae where it is in units of ph $cm^{-2}s^{-1}line^{-1}$. Multiplying by the maximum observing time (2×10^4s) we obtain column 4 which shows the ph $cm^{-2}bin^{-1}$ collected. Then, it is an easy matter to calculate column 5, the collecting area needed to achieve the desired 1000 c/bin, or for coronae, the 100 c/line.

It is apparent that, at an absolute minimum, the spectrograph should have 50 cm^2 of collecting area. This would permit the collection of good data on stellar coronae and x-ray binaries, but barely reach the Seyferts. It would fail completely on the quasars. However, with 200 cm^2 the Seyferts could be well studied, and the brightest quasars would be within reach. This higher collecting area valuable on the x-ray binaries and coronae as well, since it is less likely that variability could change the spectrum before the observation is completed, and more targets could be observed.

I recommend that the spectrograph have no less than 200 cm^2 effective collecting area.

VI. SPECTROGRAPH DESIGN

We are now faced with a very large order: Design an Explorer class instrument with resolution of 250 and collecting area of 200 cm^2. I believe it can be done, and in this section I outline one possible design.

The first point to recognize is that we must use dispersive spectroscopy coupled with grazing incidence optics. All alternatives simply will not produce the required performance. Crystal spectrographs will not achieve the necessary collecting area in a reasonable size payload because crystals operate by absorbing the great bulk of the incident photons. Solid state spectroscopy has low resolution (180eV versus the 2eV required), and there is no foreseeable chance that it will achieve high resolution during this generation. The only other alternative is dispersive spectroscopy.

In the soft x-rays we have the choice of either transmission gratings or reflection gratings for the dispersive element. There are arguments in favor of each of these which I do not wish to pursue here. I will merely say that I

personally believe that in the future x-ray astronomers, like optical astronomers, will perform virtually all their spectroscopy with reflection gratings. Reflection gratings offer higher efficiency, greater stability and higher dispersion - all properties of central importance to achieving high spectral resolution.

I have been investigating in the laboratory the level of efficiency one can expect from reflection gratings. Figure 4 shows the result obtained on a gold coated grating at 13 Å (Cash and Kohnert, 1981). This grating, replicated from a 6000 ℓ/mm, 21^0 blaze master, was ruled by Hyperfine, Inc. to make an optical element for the High Resolution Spectrograph on Space Telescope. It shows a peak efficiency of 40% in first order. With a nickel coating this would have been closer to 50%. Such very high efficiency is critical to achieving the 200 cm^2.

In addition, it is necessary to keep the number of elements in the optical train to an absolute minimum. With this is mind I have been working on the concept of the Objective Reflection Grating Spectrograph (ORGS), which, coincidentally, maximizes spectral resolution. It is quite simple, requiring only that an array of reflection gratings be mounted in front of an x-ray telescope such that the telescope views the surface of the gratings.

I have joined in a collaborative effort with Dr. Richard Catura of the Lockheed Palo Alto Research Laboratory and Dr. J.L. Culhane of the Mullard Space Sciences Laboratory to build an ORGS. We are modifying their existing telescope to hold an array of reflection gratings as shown in Figure 5. It is an Aries class telescope, and we hope to obtain our first spectrum from a rocket flight in one to two years.

It can be shown that the resolution ($\lambda/\Delta\lambda$) of an ORGS is given by

$$R = \frac{n\lambda}{d\cdot B}$$

where n is the order number, λ the wavelength, d the grating ruling spacing, and B the telescope resolution in radians. We take the best telescope resolution consistent with an Explorer mission and a proportional counter detector to be 20" ($B = 10^{-4}$). The highest ruling density currently available is about $10^4 \ell$/mm or d = 1000 Å. Thus, if R = 250 we must have

$$n\lambda = 25 \text{ Å}.$$

At energies below 0.5keV we can achieve full resolution and collecting area, while above this energy we have the choice of either full collecting area and reduced resolution (1st order), or full resolution and reduced collecting area (higher orders). This is not an ideal situation, but it is adequate.

The telescope needed to support this concept is of reasonable size. To achieve a 200 cm^2 spectrograph, we need a telescope with an effective area of 400 cm^2. A telescope the same size as ROSAT will suffice, but the mirrors need only perform at the 20" level. A proportional counter with .125 mm resolution is adequate, although one might hope that some other efficient, imaging detector might become available.

We conclude by pointing out that objective gratings cannot perform well on extended sources. There is a possible solution. A 1 x 30 arcminute collimator mator could be mounted in front of the gratings, allowing study of extended objects with R = 80.

VII. SUMMARY

I have demonstrated that in order for x-ray spectroscopy to become a serious tool of astronomy, we need to build a spectrograph with resolution in excess 250 and collecting area in excess 200 cm^2. I have presented the ORGS concept, which I believe is the easiest way to achieve these stringent specifications.

I wish to thank R. Catura and M. Shull for help in preparing this talk. I acknowledge support from NASA grant NAG5-96.

TABLE 1: TARGET FLUXES

	FLUX 10th BRIGHTEST (IPC COUNTS)	ph $cm^{-2}s^{-1}bin^{-1}$ (R = 200)	in 2×10^4s ph $cm^{-2}bin^{-1}$	cm^2 needed for 1000 ph/bin or 100 ph/line
X-RAY BINARIES	30	1.5×10^{-3}	30	30
SEYFERTS	3	1.5×10^{-4}	3	300
QUASARS	0.2	1×10^{-5}	0.2	5000
STELLAR CORONAE	1	1×10^{-4}	2	50
		ph $cm^{-2}s^{-1}line^{-1}$	ph $cm^{-2}line$	

REFERENCES

Cash, W. and Kohnert, R. 1981 Appl. Opt., in press.

Charles, P.A., et al., 1979, Ap. J. (Letters), 230, L83.

Kahn, S.M. and Blissett, R.J. 1980, Ap. J., 238, 417.

Kahn, S.M., Charles, P.A., Bowyer, S. and Blissett, R.J. 1981, Ap. J., in press.

Rappaport, S. 1979, in "Compact Galactic X-ray Sources," ed. F. Lamb and D. Pines, p. 181.

Rowland, H.A. 1882 Phil. Mag., 13, 469.

FIGURE CAPTIONS

FIGURE 1: A synthetic x-ray spectrum is shown smoothed to various resolutions: a) 280eV; b) 180; c) 64; d) 32; e) 16; f) 8; g) 4; h) 2eV. See text for discussion.

FIGURE 2: The synthetic spectrum with 2eV is shown randomized by poisson statistics with increasing number of photons.

FIGURE 3: The effect of Poisson statistics on a line spectrum is investigated.

FIGURE 4: 13A efficiency of a 6000 ℓ/mm reflection grating is shown as a function of graze angle.

FIGURE 5: Schematic of an Objective Reflection Grating Spectrograph

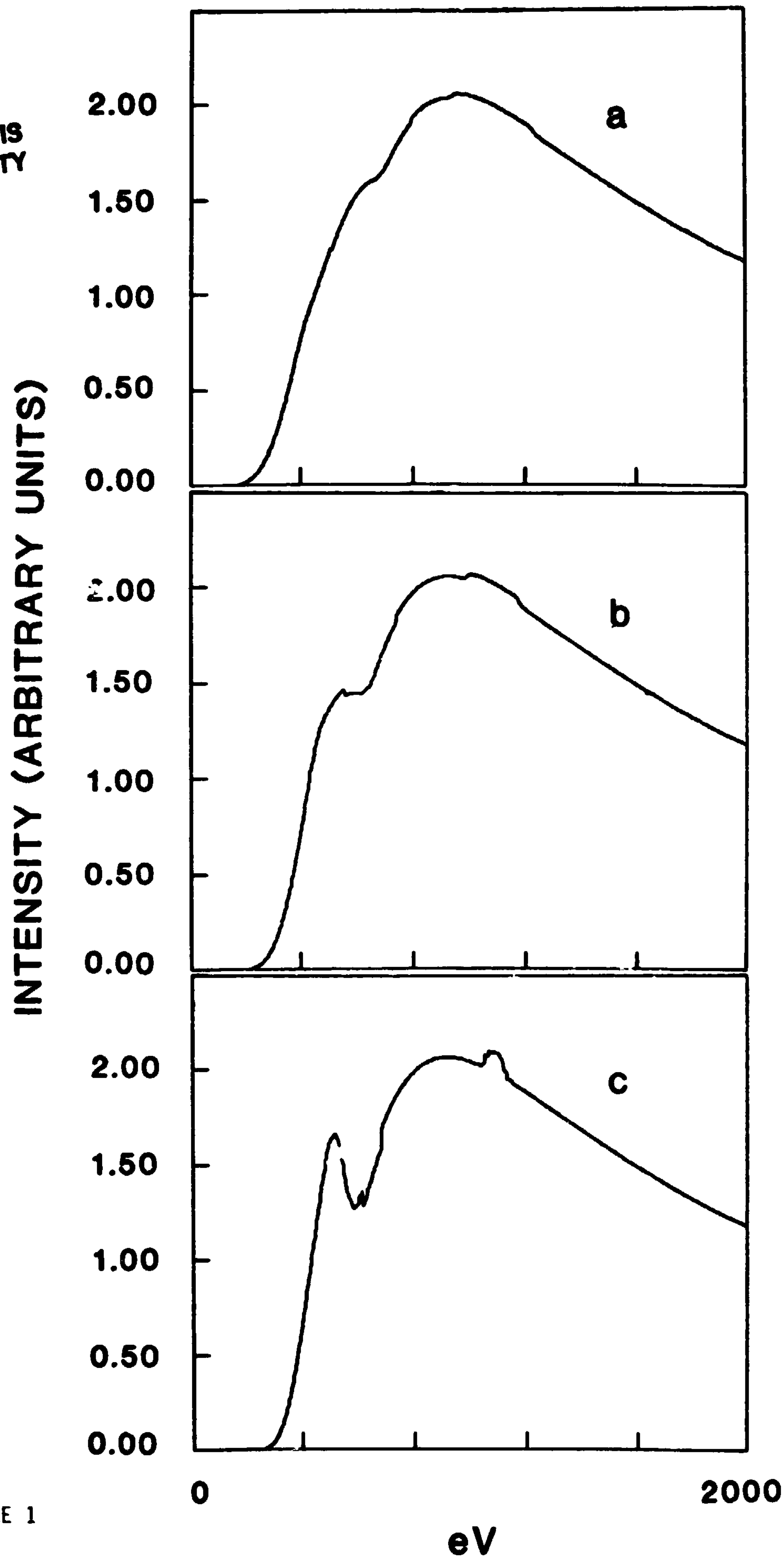
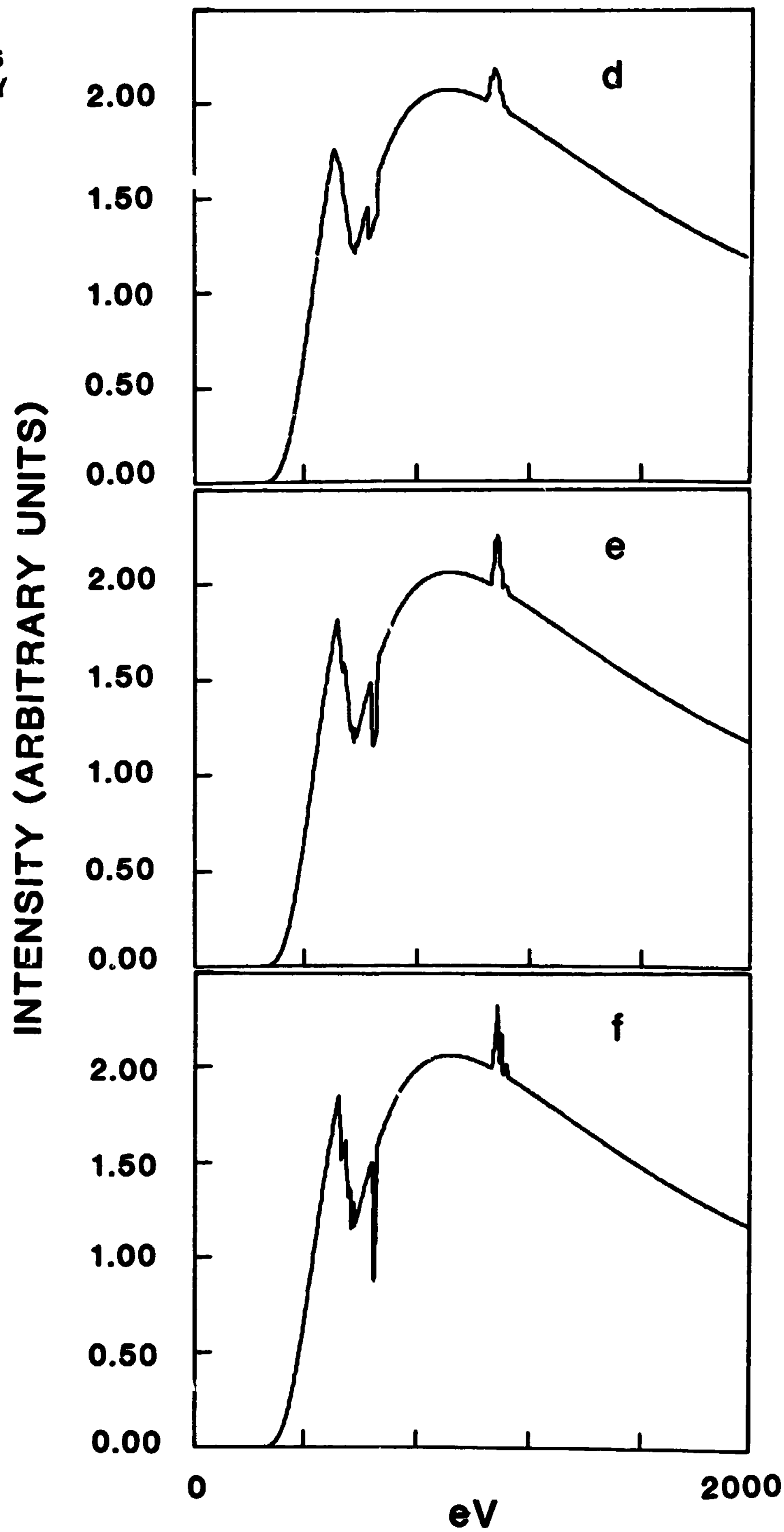
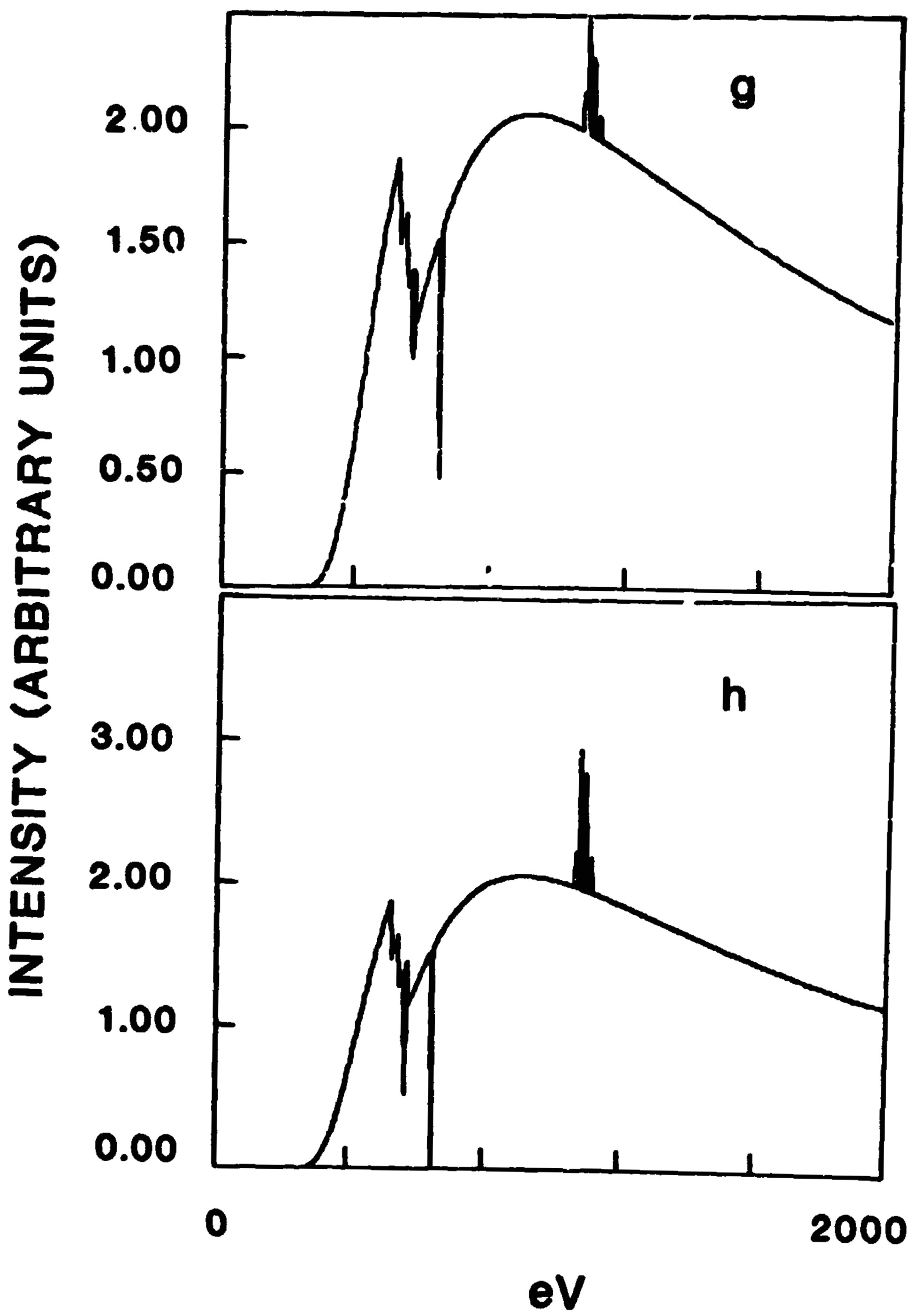


FIGURE 1


d
e
f
2.00
1.50
1.00
0.50
0.00
INTENSITY (ARBITRARY UNITS)
0
2000
eV


g
h
INTENSITY (ARBITRARY UNITS)
2.00
1.50
1.00
0.50
0.00
3.00
2.00
1.00
0.00
0
2000
eV

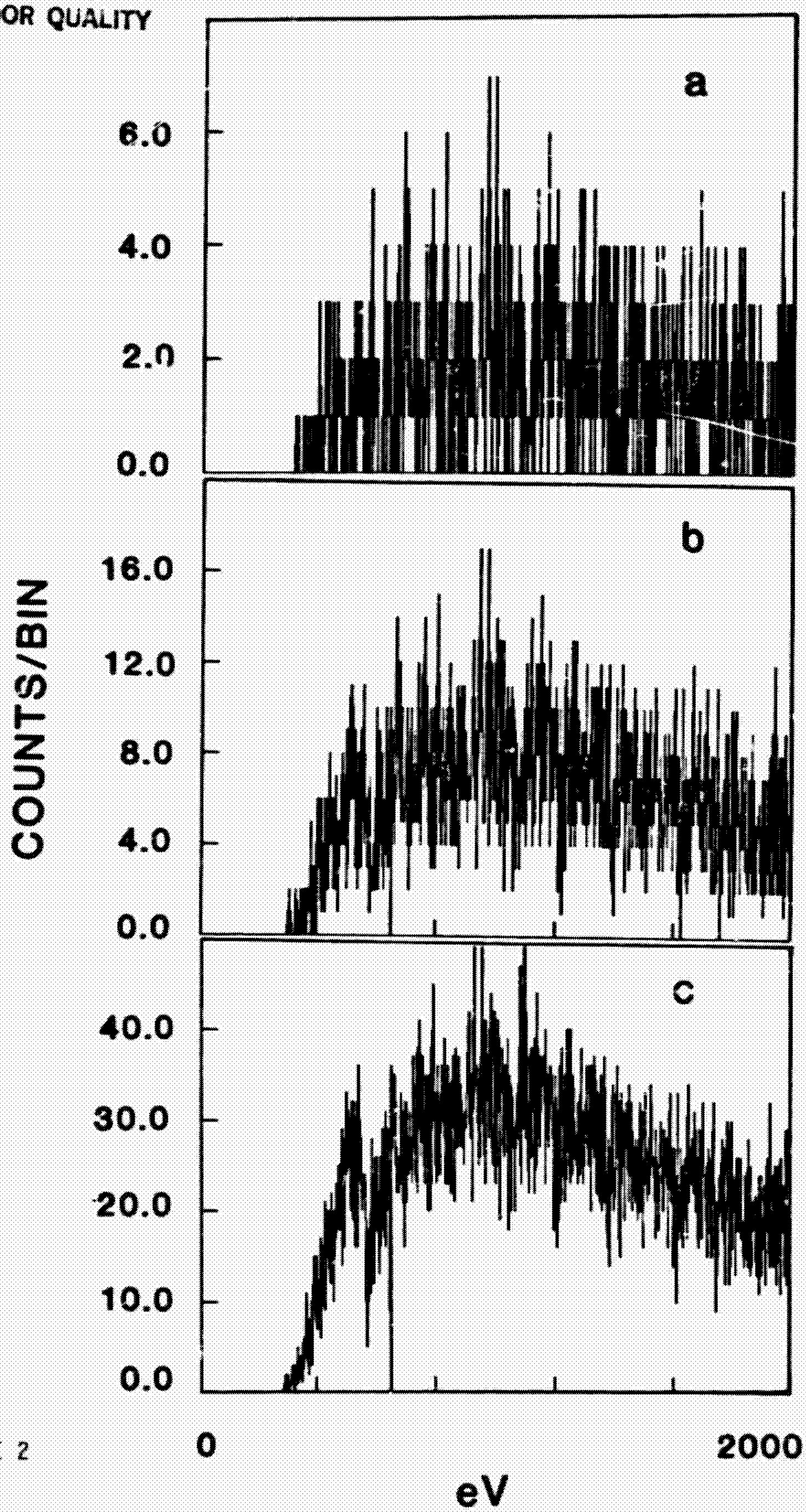
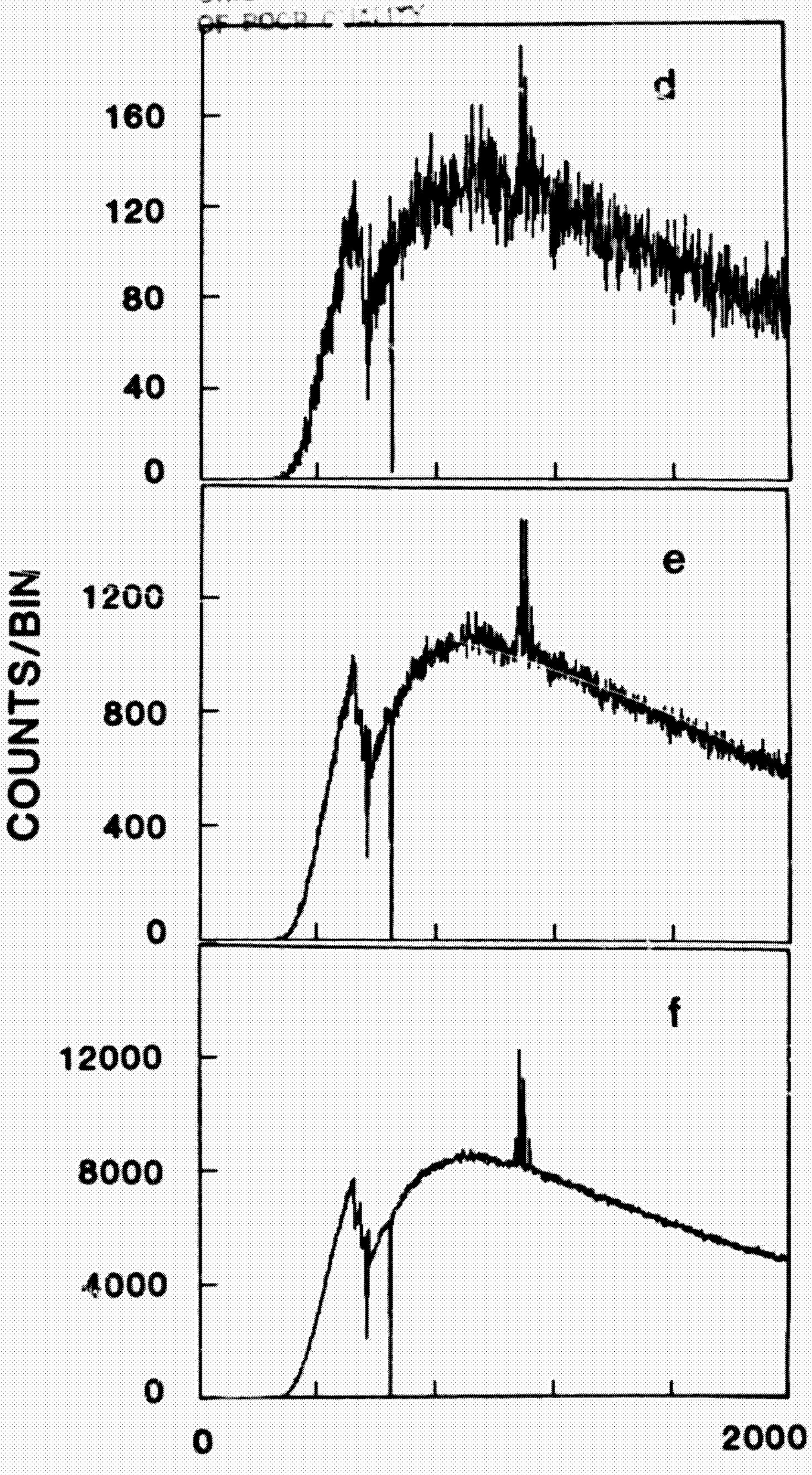

a
6.0
4.0
2.0
0.0
b
16.0
12.0
8.0
4.0
0.0
c
40.0
30.0
20.0
10.0
0.0
COUNTS/BIN
0
2000
eV

FIGURE 2


d
160
120
80
40
0
e
1200
800
400
0
f
12000
8000
4000
0
COUNTS/BIN
0
2000
eV

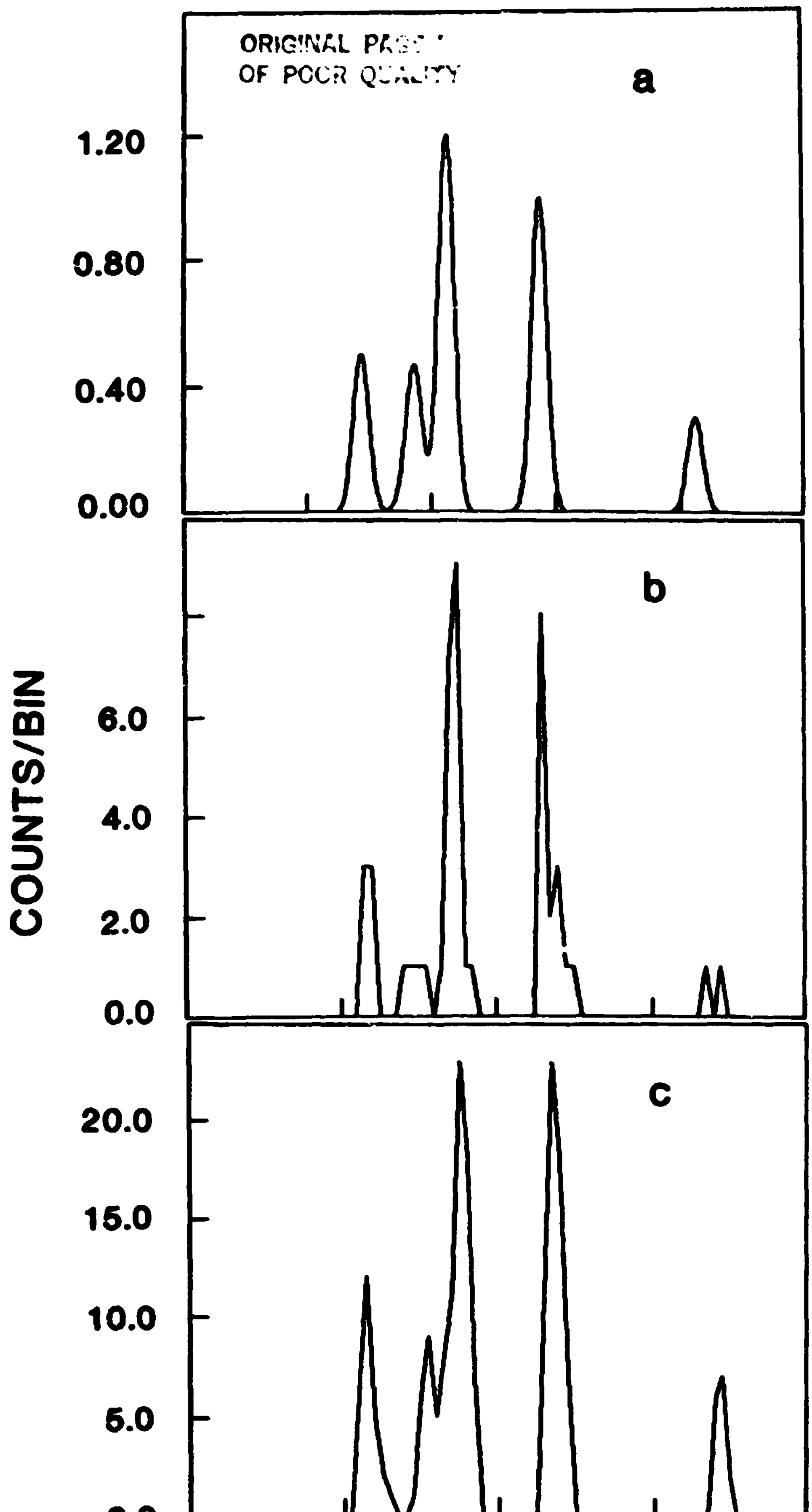
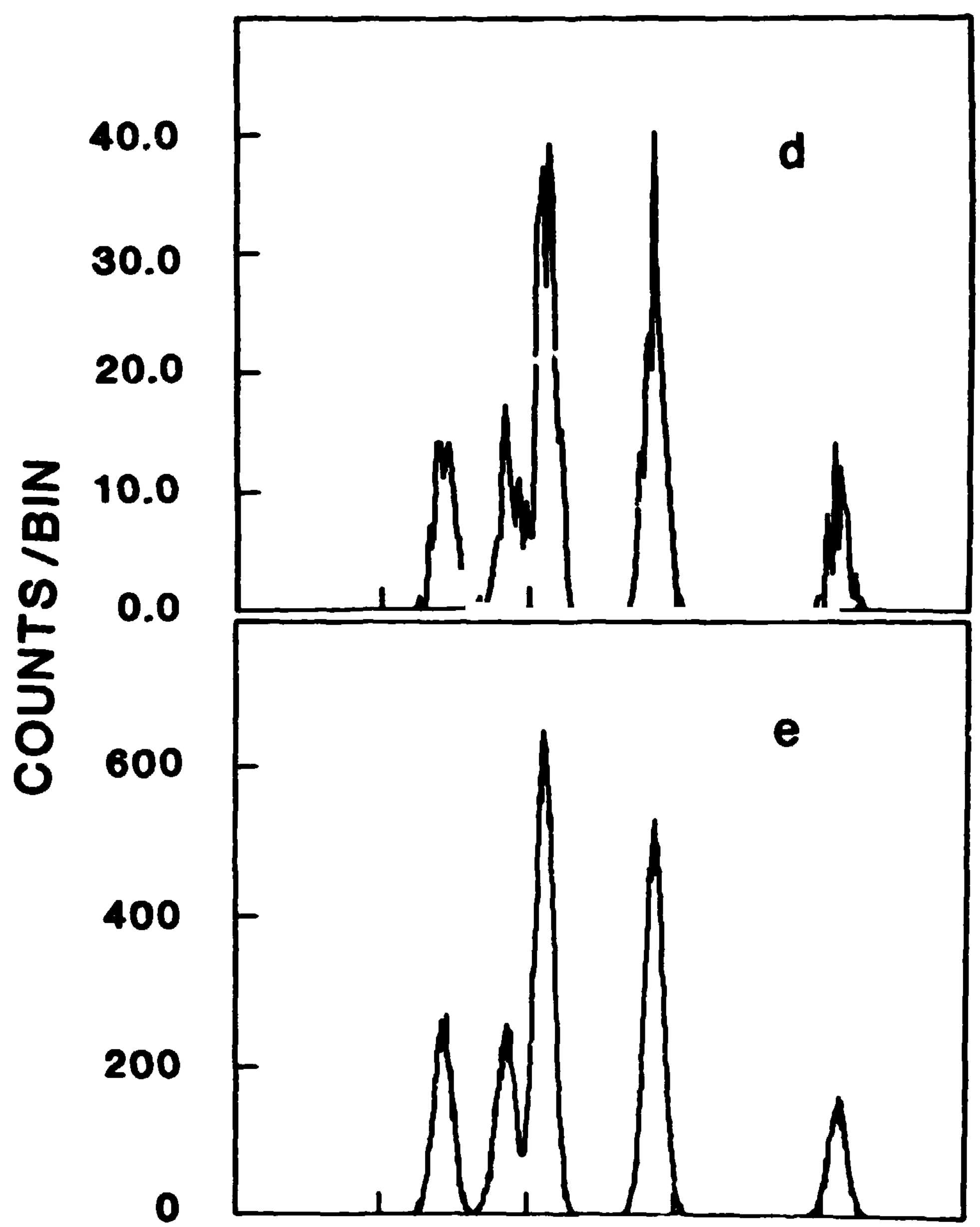

ORIGINAL PAGE IS
OF POOR QUALITY
a
1.20
0.80
0.40
0.00
b
6.0
4.0
2.0
0.0
COUNTS/BIN
c
20.0
15.0
10.0
5.0
0.0

FIGURE 3


COUNTS/BIN
40.0
30.0
20.0
10.0
0.0
d
600
400
200
0
e

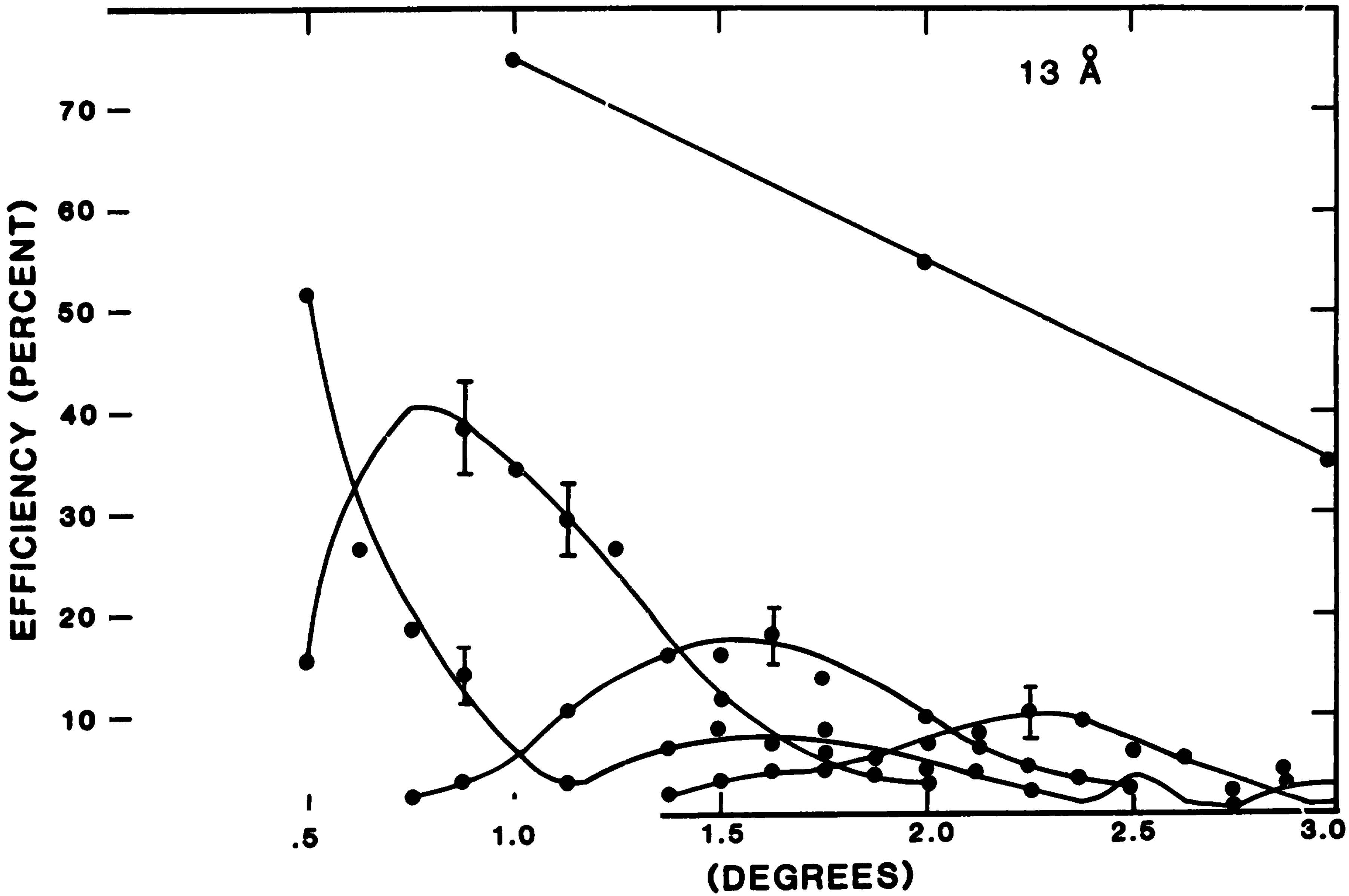

13 Å
EFFICIENCY (PERCENT)
70
60
50
40
30
20
10
.5
1.0
1.5
2.0
2.5
3.0
(DEGREES)

FIGURE 4

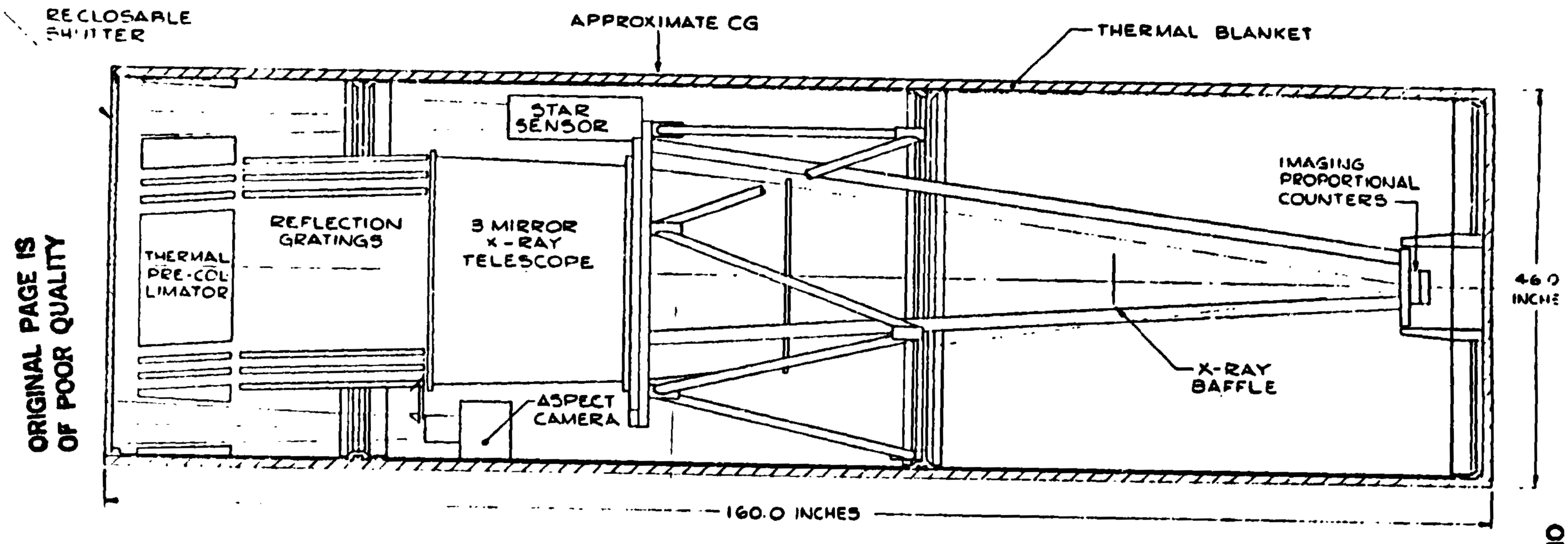


FIGURE 5

ORIGINAL PAGE IS OF POOR QUALITY